

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 147 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.60e-01

Confidence level: 7.38e-01

Nearest Neighbors from the Training Set

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Isopropylpropylamide

Measured: 148

Predicted: 173

Image not found

N-(1,1-dimethyl-2-propynyl)-4-methoxybenzamide

Measured: 67.6

Predicted: 72.5

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MCPB

Measured: 537

Predicted: 245

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4,4'-Thiodianiline

Measured: 110

Predicted: 116